

An Evaluation of Isotope Coefficient Exponent ' α ' of High T_c Superconductors

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ABSTRACT

Using the theoretical model of S. Yoksan (Solid State Commun. 78, 436 (1991)), we have studied the isotope effect in high T_c superconductors. This model takes into account the nearest neighbor interlayer hopping. Our theoretical results indicate that the value of isotope exponent α of high T_c superconductor is very small.

Keywords: Isotope effect, critical exponent, nearest neighbor interlayer hopping, high T_c - Superconductor.

INTRODUCTION

One of the most interesting experimental properties of high T_c superconductors is the small isotope effect. The suppression of this effect is not explained with the conventional BCS theory predicts that the critical temperature T_c and the isotope mass M are related by $T_c M^{-\alpha}$, where $\alpha = 0.5$ for all elements.¹⁻³

To explain the almost absence of the isotope effect in high T_c compounds, many authors have proposed various mechanisms including resonating valence bond,⁴ excitons,⁵ plasmons⁶ and antiferromagnetic spin fluctuation mediated pairing.⁷ Fund and

Kwok⁸ suggested a local volume change due to oxygen deficiency as a cause of this effect. Su et.al.⁹ interpreted experimental data as evidence for the free carrier negative U-centre interaction, Seki and Tanabe¹⁰ investigated the influence of the singularity enhanced density of states in a bond asymmetric high T_c material. Daemen and Overhauser¹¹ surprisingly found that the existence of a short range attraction in addition to the conventional phonon pairing interaction suppresses the isotope effect significantly at high temperatures.

In these calculations the authors assumed the constant electronic density of states at the Fermi level. As is well known,

high temperature superconductors have a two dimensional structure. Various calculations¹²⁻¹⁷ shows that there is a logarithmic singularity in density of states, one therefore expects that this singularity plays a dominant role in causing the anomalous behavior of the isotope effect.

Theoretical Formulation

Using the theoretical model given by Daemen and Overhauser¹¹ one assumes that the pairing interaction written as

$$V_{kk'} = \begin{cases} -V_1 - V_2, & \text{for } 0 < E < \hbar\omega_D \\ -V_2 & \text{for } \hbar\omega_D < E < 4t \end{cases} \quad (1)$$

is independent of the phonon frequency. Here V_1 is the phonon mediated interaction and V_2 is the extra interaction which may be of non electron phonon origin. E is the electron energy measured from the Fermi energy, ω_D is the Debye cut-off energy and $4t$ is the energy cut-off for V_2 .

As it has been shown by experiments that in the oxide superconductors the carriers is still the Copper pair, one thereby assumes that a solution of the BCS integral equation

$$\Delta(k) = \frac{1}{2} \sum_q \frac{V(k-q)\Delta(q)}{\sqrt{E^2 + \Delta^2(q)}} \tanh \frac{\sqrt{E^2 + \Delta^2(q)}}{2k_B T} \quad (2)$$

Based on equation (1) has the following form

$$\Delta(k, T) = \begin{cases} \Delta_0(T)\Delta_1, & \text{if } E < \hbar\omega_D \\ \Delta_0(T)\Delta_2, & \text{if } E > \hbar\omega_D \end{cases} \quad (3)$$

Here Δ_1 and Δ_2 are temperature independent constants. Upon substituting equation (3) into (2), one obtains the following equations

$$\begin{aligned} \Delta_0 \left[1 - (V_1 + V_2) \sum_1 (T) \right] &= \Delta_2 V_2 E_2(T) \\ \Delta_1 V_2 E_1(T) &= \Delta_2 [1 - V_2 E_2(T)] \end{aligned} \quad (4)$$

when

$$\begin{aligned} E_1(T) &= \int_0^{\hbar\omega_D} \frac{dEN(E)}{\sqrt{E^2 + \Delta_0^2 \Delta_1^2}} \tanh \frac{\sqrt{E^2 + \Delta_0^2 \Delta_1^2}}{2k_B T} \\ E_2(T) &= \int_{\hbar\omega_D}^{4t} \frac{dEN(E)}{\sqrt{E^2 + \Delta_0^2 \Delta_2^2}} \tanh \frac{\sqrt{E^2 + \Delta_0^2 \Delta_2^2}}{2k_B T} \end{aligned} \quad (5)$$

One obtains equation (5) by replacing the summation over q by the energy integrals.

Now in the Hubbard model on a two-dimensional square lattice, the Hamiltonian is

$$H = \sum_{ij\sigma} t C_{i\sigma}^\dagger + C_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \quad (6)$$

here t denotes the transfer integral, and U the renormalized on site Coulomb interaction, the number operation $n_{i\sigma} = C_{i\sigma}^\dagger C_{i\sigma}$. In case of the nearest neighbor hopping, the band energy is $E(k) = -2t(\cos k_x + \cos k_y)$. This gives rise to the density of states in the form

$$N(E) = \begin{cases} \frac{1}{2\pi^2 t} K \left[1 - \left(\frac{E}{4t} \right)^2 \right] & |E| < 4t \\ 0 & |E| > 4t \end{cases} \quad (7)$$

When K is the complete elliptic integral of the first kind, and $N(E)$ is non-zero only when $0 < E < 4t$, for $E \approx 0$, $N(E)$ takes the form

$$N(E) = \frac{1}{2\pi^2 t} \ln \left| \frac{E}{16t} \right| \quad (8)$$

At $T = T_c$, $\Delta_0(T) = 0$, with the aid of the expression for $N(E)$ one can see that the integrals in equation (5) are dominated around $E=0$, so one approximate equation (5) as

$$\begin{aligned} \sum_1 (T_c) &= \frac{1}{2\pi^2 t} F \left(\frac{\hbar\omega_D}{2k_B T_c} \right) \\ \sum_2 (T_c) &= -\frac{1}{2\pi^2 t} \left\{ F \left(\frac{4t}{2k_B T_c} \right) - F \left(\frac{\hbar\omega_D}{2k_B T_c} \right) \right\} \end{aligned} \quad (9)$$

With the function F defined by

$$F\left(\frac{4t}{2k_{\beta}T_c}\right) = \int_0^{\hbar\omega_D} \frac{dx \ln x}{x} \tanh\left(\frac{8tx}{k_{\beta}T_c}\right) \quad (10)$$

When equation (4) are compatible one arrives at the following condition

$$\begin{aligned} \left(\frac{\hbar\omega_D}{2k_{\beta}T_c}\right) + \sigma F\left(\frac{4t}{2k_{\beta}T_c}\right) + \lambda \sigma F\left(\frac{\hbar\omega_D}{2k_{\beta}T_c}\right) \\ \times \left[F\left(\frac{4t}{2k_{\beta}T_c}\right) - F\left(\frac{\hbar\omega_D}{2k_{\beta}T_c}\right)\right] = 0 \end{aligned} \quad (11)$$

Here one has introduced the variable $\lambda = V_1/2\pi^2t$ and $\sigma = V_2/2\pi^2t$.

T_c CALCULATION

To calculate¹³ the critical temperature T_c , one evaluates F and finds that

$$\begin{aligned} F\left(\frac{Y}{2k_{\beta}T_c}\right) = -\frac{1}{2}\ln^2\left(\frac{k_{\beta}T_c}{4t}\right) + 0.819\ln\left(\frac{k_{\beta}T_c}{8t}\right) \\ + \frac{1}{2}\ln^2\left(\frac{Y}{16t}\right) - 1 \end{aligned} \quad (12)$$

Putting F in equation (11) and rearranging, one arrives at the equation for T_c .

$$k_{\beta}T_c = 1.13\hbar\omega_D \exp\left\{\frac{1}{\lambda + \sigma^*} - \frac{0.6646}{\ln(\hbar\omega_D/16t)}\right\} \quad (13)$$

Where

$$\sigma^* = \frac{\sigma}{1 - \frac{\sigma}{2} \ln\left(\frac{4t}{\hbar\omega_D}\right) \ln\left(\frac{64t}{\hbar\omega_D}\right)} \quad (14)$$

In the pure electron-phonon mechanism, i.e.

when $V_1 \neq 0$ and $V_2 = 0$ and $\sigma = 0$ equation (13) gives.

$$k_{\beta}T_c = 1.13\hbar\omega_D \exp\left\{\frac{1}{\frac{V_1}{2\pi^2t} \ln\left(\frac{\hbar\omega_D}{16t}\right)}\right\} \quad (15a)$$

In the dominate non electron-phonon process, i.e. when $V_2 \gg V_1$, we have $\lambda \rightarrow 0$ and $\sigma \neq 0$ equation (13) gives.

$$k_{\beta}T_c = 8t \exp\left(-\sqrt{\frac{4\pi^2t}{V_2}}\right) \quad (15b)$$

Here the quantity of $1/2\pi^2t|\ln(\hbar\omega_D/16t)|$ is analogous to the density of states at the Fermi level of the BCS theory. If this quantity is large, $T_c \sim \omega_D$. Thus the logarithmic singularity yields a function $|1/\ln(\hbar\omega_D/16t)|$ giving an important enhancement of T_c .

For $V_2 \neq 0$, one calculates T, as a function of σ/λ for different ratios $\hbar\omega_D/16t$.

α CALCULATION

The isotope effect exponent can be derived from equation (13) as

$$\alpha = \frac{d \ln T_c}{d \ln M} \quad (16)$$

In the phonon-mediated pairing scheme ω_D is proportional to $M^{-1/2}$, when M is the average mass of the atom constituting the specimen under consideration, using equation (13) in equation (16), one finds

$$= \frac{1}{2} \left\{ 1 - \left[1 - \lambda \left(0.6646 + \ln \frac{\hbar\omega_D}{16t} \ln \frac{k_{\beta}T_c}{1.134\hbar\omega_D} \right) \right]^2 - \frac{\ln\left(\frac{k_{\beta}T_c}{1.134\hbar\omega_D}\right)}{\ln(\hbar\omega_D/16t)} \right\} \quad (17)$$

in the limit of low T_c , it is straight forward to show that equation (17) can be estimated as

$$\alpha = \frac{1}{2} \left\{ 1 - \left[1 - \lambda \ln \left(\frac{\hbar\omega_D}{16t} \times \ln \frac{k_\beta T_c}{1.134\hbar\omega_D} \right) \right]^2 \right\} \quad (18)$$

Here the quantity

$$\left| \frac{V_1}{2\pi^2 t} \ln \left(\frac{\hbar\omega_D}{16t} \right) \right| \quad (19)$$

in this model is equivalent to $N_0 V_1$ in equation (12).

In a refined version of α , one calculates it directly by differentiating equation (11) with respect to M and get

$$\alpha = \frac{1}{2} \left\{ \left[1 - \frac{H(\hbar\omega_D/k_\beta T_c)}{\ln \left(\frac{\hbar\omega_D}{16t} \right) \tanh \left(\frac{\hbar\omega_D}{2k_\beta T_c} \right)} \right] \times \left[1 - \frac{[1 + \lambda(\hbar\omega_D/k_\beta T_c)]^2}{\lambda F \left(\frac{\hbar\omega_D}{2k_\beta T_c} \right) \left[2 + \lambda F \left(\frac{\hbar\omega_D}{2k_\beta T_c} \right) \right]} \right] \right. \\ \left. \times \frac{\left[\ln \frac{1}{4} \tanh \frac{4t}{2k_\beta T_c} - H \left(\frac{4t}{2k_\beta T_c} \right) \right]}{\ln \left(\frac{\hbar\omega_D}{16t} \right) \tanh \left(\frac{\hbar\omega_D}{2k_\beta T_c} \right) - H \left(\frac{\hbar\omega_D}{2k_\beta T_c} \right)} \right\}^{-1}$$

were

$$H \left(\frac{y}{2k_\beta T_c} \right) = \int_0^{y/16t} \frac{dx}{x} \tanh \left(\frac{8tx}{k_\beta T_c} \right)$$

Table T₁

| High T_c Superconductor | T_c (K) | Θ_D (K) | t (K) | λ | α^{theo} | α^{expt} |
|---|-----------|----------------|---------|-----------|-----------------|----------------------|
| $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ | 37 | 240 | 5000 | 0.02 | 0.19 | 0.16 |
| $\text{YBa}_2\text{Cu}_3\text{O}_7$ | 92 | 450 | 6000 | 0.01 | 0.09 | 0.018 ± 0.004 |
| $\text{Bi}_2\text{Sr}_2\text{Ca}_2\text{Cu}_3\text{O}_{10}$ | 107 | 535 | 6925 | 0.025 | 0.048 | 0.026 ± 0.02 |
| $\text{Ba}_{0.6}\text{K}_{0.4}\text{BO}_3$ | 32 | 186 | 4783 | 0.022 | 0.40 | 0.042 ± 0.05 |
| $(\text{Tl}_{0.5}\text{Pb}_{0.5})\text{Sr}_2\text{Cu}_2\text{Cu}_3\text{O}_9$ | 122 | 639 | 7447 | 0.039 | 0.037 | 0.027 ± 0.003 |

DISCUSSION OF RESULTS

In this paper, we have studied the isotope effect in high T_c superconductor

within the conventional BCS theory. By passing that there exist the usual attractive interaction, Originating from the phonon exchange and an attractive interaction from

the unknown origin. One calculates the transition temperature T_c and the isotope effect exponent α . The possible singular behaviour in the density of states and the relative importance of the attractive interaction T_c and α are investigated. It is found that the singularity contributes to the enhancement of T_c . For high critical temperature, the second attractive interactions must be the stronger of the two. One also observes that the behaviour of the exponent α depends sensitively on the relative magnitude of the two interactions. The results are shown in table T_1 .

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